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Calculated self-energy contributions for an *ns* valence electron using the multiple-commutator method

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The self-energy (SE) correction is evaluated for a single valence *ns* electron of heavy and superheavy atoms with *n* up to 8 and the nuclear charge *Z* up to 119. The recently developed approach based on the commutator expansion is employed. Various Dirac-Slater one-electron local potentials with extended nuclei are used. The Lamb shifts were calculated by adding the average values of the Uehling potential to the SE contributions. The results confirm the earlier estimates for the quantum electrodynamical effects on the valence energies of heavy and superheavy atoms. [S1050-2947(99)07004-3]

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I. INTRODUCTION

In the preliminary communication [1], we presented estimates for the Lamb shift of the valence *ns*-electron levels in the alkali and coinage metal atoms [groups 1 (Li-Fr) and 11 (Cu-Au), respectively]. These estimates showed that the radiative corrections are not entirely negligible for the heavy and superheavy atoms, and can rise up to 0.5% of the ionization energy in the latter case. The estimates were based on the calculation of the average value of the Uehling potential for the vacuum polarization (VP) and the ratio SE/VP (SE is the self-energy) taken from the Coulomb field calculations for 1*s* and 2*s* electrons [2]. In this paper we will support these estimates by actual calculations of the SE for one *ns* valence electron in a local effective potential.

The SE contribution is now directly calculated using the newly developed multiple commutator method (MCM) [3,4] (see also Ref. [5]). This method combined with the *B*-spline numerical approach is easily applicable for electrons in any state, and moving in any local one-electron potential *V*. For calculating the SE we will use various Dirac-Slater (DS) potentials with extended nucleus.

The accuracy of the MCM can best be tested against the previous calculations on hydrogenlike systems; see Refs. [4,6,7]. That accuracy is now improved along the lines, introduced in Refs. [5,8].

To evaluate the Lamb shift the vacuum polarization corrections are added to the SE. These corrections are handled as in Ref. [1], but now include the minor effects of the finite nucleus and of the screened atomic potential.

The paper is organized as follows: the self-energy is discussed in Sec. II and the vacuum polarization in Sec. III. The three different local potentials and the resulting wave functions are deferred to the Appendix.

II. SELF-ENERGY

For the calculation of the SE contribution we apply an approach based on the multiple commutator expansion [3,4]. Within this approach the self-energy correction to the atomic state *A* looks like

$$\Delta E_{\mathrm{SE}}^{A}=\frac{\alpha}{\pi}\sum_{m}\left(\frac{1-\vec{\alpha}_1\cdot\vec{\alpha}_2}{\alpha r_{12}}I_{mA}(r_{12})\right)_{AmmA}-\delta m_A, \quad (1)$$

where $\vec{\alpha}_i$ are the Dirac matrices for the different variables, $r_{12}=|\vec{r}_1-\vec{r}_2|$. We use the notation

$$(F)_{A,B,C,D,}=\int d\vec{r}_1 d\vec{r}_2 \psi_A^{+}(\vec{r}_1)\psi_B^{+}(\vec{r}_2) \times F(\vec{r}_1,\vec{r}_2)\psi_C(\vec{r}_1)\psi_D(\vec{r}_2) \quad (2)$$

where $\psi_{A,B,C,D}$ are the solutions of the Dirac equations

$$\hat{h}(\vec{r})\psi_A^{+}(\vec{r})=E_A\psi_A^{+}(\vec{r}), \quad (3)$$

TABLE I. The SE contributions for hydrogenlike systems and finite nuclei as function of *Z* and *n* (in eV).

Z	*n*	This work	Refs. [6,7]	Deviation
10	1	0.15665	0.15660	<1%
20	1	1.74823	1.74821	<1%
20	2	0.23675	0.23538	<1%
30	1	6.95770	6.95773	<1%
30	2	0.97001	0.96737	<1%
30	3	0.28977	0.29457	1.5%
40	4	0.33505	0.33948	1.3%
50	5	0.37921	0.38427	1.3%
60	3	3.40490	3.4624	1.7%
70	3	6.1826	6.2479	1%
80	2	35.901	35.565	2%
90	2	60.990	59.861	2%
100	2	102.12	100.27	2%
100	3	30.454	29.792	2%
110	4	22.471	20.392	9%

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TABLE II. The SE contributions to the valence-electron energy levels for the alkali and coinage metal atoms (in eV). The wave functions (1)–(3) are explained in the text.

Z	System	State	(1)	(2)	(3)
3	Li	$2s$	3.84×10^{-5}	5.17×10^{-5}	5.22×10^{-5}
11	Na	$3s$	2.83×10^{-4}	4.05×10^{-4}	4.56×10^{-4}
19	K	$4s$	4.93×10^{-4}	6.92×10^{-4}	8.74×10^{-4}
37	Rb	$5s$	1.23×10^{-3}	1.66×10^{-3}	2.22×10^{-3}
55	Cs	$6s$	2.15×10^{-3}	2.72×10^{-3}	3.83×10^{-3}
87	Fr	$7s$	6.03×10^{-3}	7.07×10^{-3}	9.83×10^{-3}
119		$8s$	2.74×10^{-2}	2.97×10^{-2}	
29	Cu	$4s$	2.66×10^{-3}	3.67×10^{-3}	5.05×10^{-3}
47	Ag	$5s$	6.14×10^{-3}	7.92×10^{-3}	1.06×10^{-2}
79	Au	$6s$	2.21×10^{-2}	2.66×10^{-2}	3.21×10^{-2}
80	Hg^{+}	$6s$	3.31×10^{-2}	3.59×10^{-2}	4.09×10^{-2}
81	Tl^{2+}	$6s$	4.68×10^{-2}	4.89×10^{-2}	5.30×10^{-2}
111		$7s$	8.66×10^{-2}	9.46×10^{-2}	

$$\hat{h}(\vec{r})=\frac{\vec{\alpha}\cdot\vec{p}}{\alpha}+\frac{\beta}{\alpha^2}+V(\vec{r}). \tag{4}$$

$\vec{p}=-i\vec{\nabla}$, β is the Dirac matrix, $V(\vec{r})$ is an arbitrary local potential, and E_A is the Dirac eigenvalue. Here we use the atomic units ($e=m_e=\hbar=1$, $c=1/\alpha$). The sum in Eq. (1) is extended over the complete Dirac spectrum for the bound electron.

The function $I_{mA}(r_{12})$ is defined as

$$I_{mA}(r_{12})=\ln\alpha^2|E_m-E_A|\sin[(E_m-E_A)\alpha r_{12}]+\frac{\pi}{2}\frac{|E_m|}{E_m}\cos[(E_m-E_A)\alpha r_{12}]. \tag{5}$$

The counterterm we define as

$$\delta m_A=\frac{\alpha}{\pi}\int d\vec{p}\,|\langle\psi_A(\vec{r})|\psi_{\vec{p}}(\vec{r})\rangle|^2\times\int d\vec{q}\left(\frac{1-\vec{\alpha}_1\cdot\vec{\alpha}_2}{\alpha r_{12}}I_{\vec{p}\cdot\vec{q}}(r_{12})\right)_{\vec{p},\vec{q},\vec{q},\vec{p}}, \tag{6}$$

where $\psi_A(\vec{r})$ are Dirac eigenfunctions in the coordinate representation, and $\psi_{\vec{p}}$ are the spherical wave solutions of the Dirac equation for the free electron, described by the Dirac Hamiltonian (4) with $V=0$. Integration over $\vec{p}$ is interpreted as integration over the energies $E_p=\pm(1/\alpha)\sqrt{p^2+1/\alpha^2}$, where p is the absolute value of the electron momentum. The summations over angular momentum numbers are also understood. The same expression for $\Delta E_{\mathrm{SE}}^{A}$ with the use of the multiple commutator expansion [3] was derived also in Ref. [5].

In the previous calculation [4], the values for the counterterm were obtained analytically because the radial integrals over r_1 and r_2 contain three Bessel functions and are well known, and the angular part of the calculation is performed in the standard way. After this the integration over $\vec{p}$ and $\vec{q}$ can be done numerically.

TABLE III. Effects of electronic screening on the calculated VP contribution, eV. The Dirac-Fock level is used for the many-electron systems. Finite nuclear models are assumed.

Z	System	State	E_{VP}	
			Unscreened	Screened
92	U^{89+}	$2s$	-15.789 -15.7722 [8]	-15.748 -15.7315 [8]
3	Li	$2s$	-1.38×10^{-6}	-1.36×10^{-6}
11	Na	$3s$	-1.54×10^{-5}	-1.52×10^{-5}
19	K	$4s$	-3.43×10^{-5}	-3.42×10^{-5}
37	Rb	$5s$	-1.31×10^{-4}	-1.31×10^{-4}
55	Cs	$6s$	-2.99×10^{-4}	-2.99×10^{-4}
87	Fr	$7s$	-1.43×10^{-3}	-1.43×10^{-3}
119		$8s$	-1.01×10^{-2}	-1.01×10^{-2}
29	Cu	$4s$	-2.36×10^{-4}	-2.36×10^{-4}
47	Ag	$5s$	-7.34×10^{-4}	-7.34×10^{-4}
79	Au	$6s$	-4.62×10^{-3}	-4.62×10^{-3}
111		$7s$	-3.19×10^{-2}	-3.19×10^{-2}

For obtaining a higher accuracy within the B-spline [9] method, following Ref. [5] we can rewrite the counterterm in Eq. (1) as

$$\delta m_A=\frac{\alpha}{\pi}\sum_{p}|\langle\psi_A|\psi_{\vec{p}}\rangle|^2\sum_{q}\left(\frac{1-\vec{\alpha}_1\cdot\vec{\alpha}_2}{\alpha r_{12}}I_{\vec{p}\cdot\vec{q}}(r_{12})\right)_{\vec{p},\vec{q},\vec{q},\vec{p}}, \tag{7}$$

where Σ_p and Σ_q denote the summations over the spline Dirac spectrum at the limit $Z\rightarrow0$. This leads to the cancellation of the spline inaccuracies.

As a test of the accuracy of the SE, calculated with Eq. (7), in Table I we give the results for one-electron systems. For the n values available and $Z<90$ the deviation from Mohr and co-workers' values [6,7] is less than 2%.

The E_{SE} for the valence electron of many-electron systems are given in Table II. Three different electronic wave functions are used: (1) Dirac-Fock, (2) Dirac-Slater with α_x fitted to $\varepsilon_{ns}=\varepsilon_{ns}^{\mathrm{DF}}$, and (3) Dirac-Slater with α_x fitted to

TABLE IV. Vacuum-polarization energies in eV. The wave functions (1)–(3) are explained in the text.

Z	System	State	(1)	(2)	(3)
3	Li	$2s$	-1.38×10^{-6}	-1.73×10^{-6}	-1.75×10^{-6}
11	Na	$3s$	-1.54×10^{-5}	-2.19×10^{-5}	-2.47×10^{-5}
19	K	$4s$	-3.43×10^{-5}	-4.73×10^{-5}	-6.06×10^{-5}
37	Rb	$5s$	-1.31×10^{-4}	-1.72×10^{-4}	-2.30×10^{-4}
55	Cs	$6s$	-2.99×10^{-4}	-3.75×10^{-4}	-5.28×10^{-4}
87	Fr	$7s$	-1.43×10^{-3}	-1.63×10^{-3}	-2.26×10^{-3}
119		$8s$	-1.01×10^{-2}	-1.09×10^{-2}	
29	Cu	$4s$	-2.36×10^{-4}	-3.21×10^{-4}	-4.38×10^{-4}
47	Ag	$5s$	-7.34×10^{-4}	-9.44×10^{-4}	-1.26×10^{-3}
79	Au	$6s$	-4.62×10^{-3}	-5.42×10^{-3}	-6.52×10^{-3}
80	Hg^{+}	$6s$	-7.03×10^{-3}	-7.44×10^{-3}	-8.41×10^{-3}
81	Tl^{2+}	$6s$	-9.67×10^{-3}	-1.01×10^{-2}	-1.10×10^{-2}
111		$7s$	-3.20×10^{-2}	3.36×10^{-2}	

TABLE V. The Lamb shift calculations for the valence electrons in the alkali and coinage metal atoms, eV. The wave functions (1)–(3) are explained in the text.

			Total Lamb shift				
Z	System	State	Ratio method [1]	This work			Other methods
			DF	(1)	(2)	(3)	
3	Li	$2s$	3.991×10^{-5}	3.70×10^{-5}	5.00×10^{-5}	5.05×10^{-5}	3.049×10^{-5} [a]
11	Na	$3s$	2.759×10^{-4}	2.68×10^{-4}	3.83×10^{-4}	4.32×10^{-4}	
19	K	$4s$	4.729×10^{-4}	4.59×10^{-4}	6.44×10^{-4}	8.13×10^{-4}	
37	Rb	$5s$	1.195×10^{-3}	1.10×10^{-3}	1.49×10^{-3}	1.99×10^{-3}	
55	Cs	$6s$	1.923×10^{-3}	1.85×10^{-3}	2.35×10^{-3}	3.30×10^{-3}	
87	Fr	$7s$	4.754×10^{-3}	4.60×10^{-3}	5.44×10^{-3}	7.58×10^{-3}	
119		$8s$	1.752×10^{-2}	1.73×10^{-2}	1.88×10^{-2}		
29	Cu	$4s$	2.543×10^{-3}	2.42×10^{-3}	3.35×10^{-3}	4.61×10^{-3}	
47	Ag	$5s$	5.506×10^{-3}	5.40×10^{-3}	6.98×10^{-3}	9.32×10^{-3}	
79	Au	$6s$	1.842×10^{-2}	1.75×10^{-2}	2.12×10^{-2}	2.55×10^{-2}	
80	Hg^{+}	$6s$		2.61×10^{-2}	2.85×10^{-2}	3.25×10^{-2}	
81	Tl^{2+}	$6s$		3.71×10^{-2}	3.87×10^{-2}	4.20×10^{-2}	
111		$7s$	5.656×10^{-2}	5.47×10^{-2}	6.10×10^{-2}		

[a] Reference [15], discussed in the text.

$\varepsilon_{ns} = -I$ (α_x is the Slater exchange parameter, and I is the experimental first ionization potential). Cases (2) and (3) could be run with or without the Salvat parametrization [10] with identical results. Case (1) also could be fitted to a local potential to high accuracy.

III. VACUUM POLARIZATION

The dominant vacuum polarization term arises from the Uehling potential. This term alone gives more than 90% of the total VP contribution for an ns shell in the case of the hydrogenlike ions [8,11]. The VP effect is dominated by the strong Coulomb field near nucleus. Therefore we can expect that the Uehling potential term will suffice in the screened systems as well. Thus within the inaccuracy of the SE calculation we can treate the VP in the Uehling approximation.

We now calculate the VP part using the Uehling approximation for an extended nucleus, as done in Refs. [12–14]. For the nuclear charge distribution $\rho_{\mathrm{nucl}}(r)$ we will use the model of the uniformly charged sphere. We designate the corresponding VP potential as $V^{\mathrm{C}}_{\mathrm{Ue,ext}}$. We can estimate the effects of atomic screening by replacing the nuclear charge distribution $\rho_{\mathrm{nucl}}(r)$ by

$$\rho(r) = \rho_{\mathrm{nucl}}(r) + \rho_{\mathrm{c}}(r), \tag{8}$$

where $\rho_{\mathrm{c}}(r)$ is the core electron density.

In Table III we see that for Li-like U Eq. (8) gives a result that agrees with that of Persson *et al.* [14]. Second, it is seen that for the lightest neutral atom, Li, the electronic screening effects diminish E_{VP} by 1%. For the valence electrons of the heavier alkali atoms the electronic screening effects on E_{VP} become even smaller; see Table III. The final results for the VP contribution are given in Table IV for the three approximations mentioned above.

The total Lamb shifts are given in Table V, and the $-E_{\mathrm{SE}}/E_{\mathrm{VP}}$ ratios in Table VI. We include for reference the ratios for the Coulombic $2s$ level from Johnson and Soff [2]. From the latter table we can see that the model-potential and Coulombic ratios are very similar. Thus the ''ratio method'' for the SE in Ref. [1] was reasonable.

Our values for the Lamb shift of the $2s$ electron of lithium range from 3.70×10^{-5} eV at the Dirac-Fock (DF) level to 5.05×10^{-5} eV in the DS (ionization potential) model. The latest literature value is that by Yan and Drake [15], 3.049×10^{-5} eV, using a highly correlated atomic wave function. While the comparison of absolute Lamb shifts is hampered by correlation effects, the ratio of the Lamb shift to the kinetic relativistic effects is very similar, -8.48×10^{-2} and -8.75×10^{-2} for our DF case (1) and the correlated calculation [15], respectively. Apart from the Li $2s$ Lamb shift, we are not aware of other earlier results on neutral, or nearly neutral atoms, that could be used to test our results (see Fig. 1).

TABLE VI. The ratios $-E_{\mathrm{SE}}/E_{\mathrm{VP}}$. The wave functions (1)–(3) are explained in the text. The last column is Coulombic.

Z	System	State	This work			Ref. [2]
			(1)	(2)	(3)	($2s$)
3	Li	$2s$	27.61	29.89	29.88	29.71
11	Na	$3s$	18.25	18.50	18.50	18.80
19	K	$4s$	14.29	14.61	14.42	14.70
37	Rb	$5s$	9.343	9.690	9.655	10.08
55	Cs	$6s$	7.180	7.261	7.260	7.427
87	Fr	$7s$	4.227	4.329	4.359	4.335
119		$8s$	2.715	2.716		2.722
29	Cu	$4s$	11.22	11.43	11.53	11.73
47	Ag	$5s$	8.333	8.393	8.399	8.476
79	Au	$6s$	4.991	4.912	4.913	4.991
80	Hg^{+}	$6s$	4.712	4.832	4.859	4.906
81	Tl^{2+}	$6s$	4.842	4.828	4.831	4.822
111		$7s$	2.723	2.815		2.780

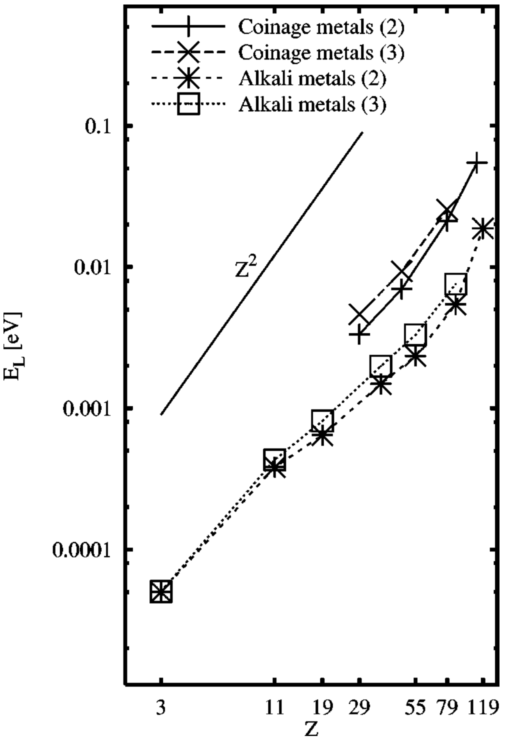

FIG. 1. Total Lamb shifts in the DS approximations (2) $[\varepsilon_{ns}=\varepsilon(\mathrm{DF})]$ and (3) $(\varepsilon_{ns}=-IP_1)$.

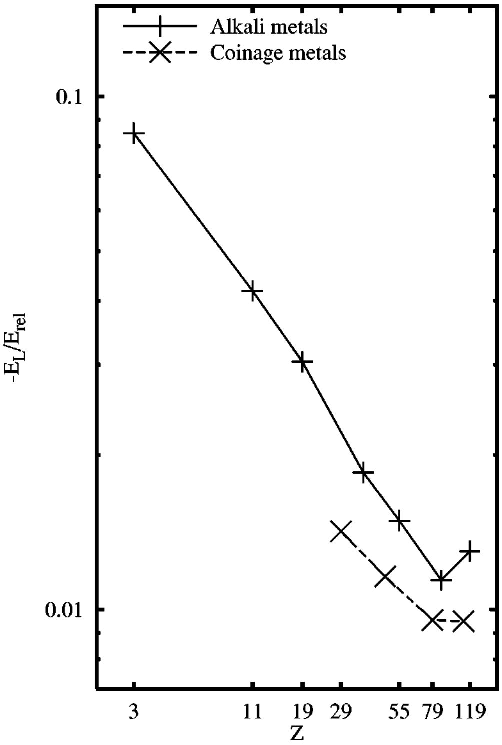

FIG. 2. The ratios of the Lamb shift to the relativistic contribution for the alkali and coinage metals at Dirac-Fock level.

Our calculated Lamb shifts for the 6s electron of Tl^{2+} are 4×10^{-2} eV. The deviation of the best calculated $6s\rightarrow6p_{1/2,3/2}$ energies from experiment are 0.063 and 0.074 eV, respectively [16]. Thus somewhat more accurate calculations will be needed to see the Lamb shift.

IV. CONCLUSIONS

The previous calculations [1] were based on the assumptions that the SE/VP ratio is the same for H-like atoms and the valence electron of neutral alkali and coinage metals. From Table V we now see that this was a very good approximation. If one assumes that the SE effects behave like the VP ones and mainly come from the range $r\sim10^{-3}$ a.u. [1], where the potential is almost Coulombic, this might be expected. Because the total field ''seen'' by the ns electron is strongly non-Coulombic, the SE results had to be checked, however. The absolute values of the valence-electron Lamb shift depend on the effective valence-electron density near the nucleus.

The question may arise of whether there are no other small contributions not taken into account here and comparable in magnitude to the first-order QED corrections considered. First, there are two-electron QED corrections partly included in our VP and SE calculations due to the use of the screened one-electron wave functions in Eq. (1) and the screened density in the VP. The remaining two-electron QED corrections are at least one order of magnitude smaller [17]. The second-order QED corrections are two orders of magnitude smaller [18].

Even smaller contributions arise from the muonic (pionic, etc.) loop corrections or the parity-conserving weak-interaction corrections [18]. Among the non-QED corrections the most important one is the nuclear size correction that even dominates over the QED corrections for very high-Z values [1]. The uncertainty in the determination of the nuclear radius sets the principal limit to the *ab initio* calcu-

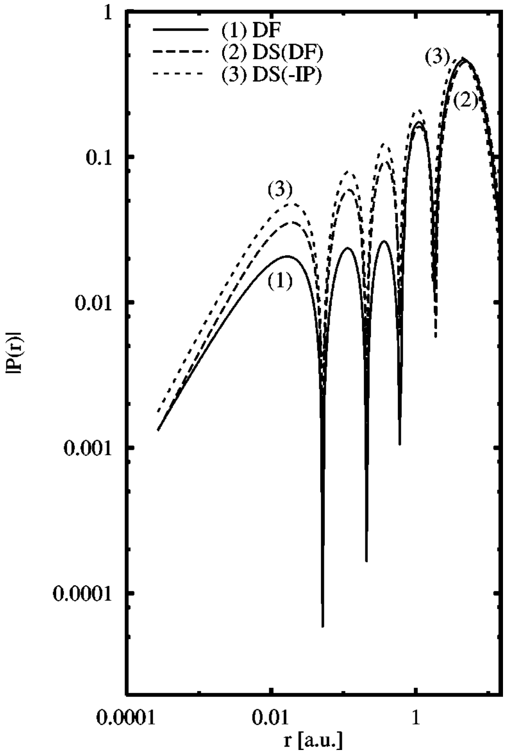

FIG. 3. The absolute value of the large component, $|P(r)|$, for the 5s valence orbital of rubidium ($Z=37$) in the DF approximation (1) and the DS approximations (2) and (3).

TABLE VII. Relativistic correction factors R/NR for magnetic dipole hyperfine integrals $M1$ [21], the Uehling potential VP, and the Mössbauer isomer shift S' [22].

Z	System	State	Ratio R/NR			
			$M1$(H-like)	$M1$(DF)	VP(DF)	S'(H-like)
29	Cu	$4s$	1.1011	1.1507	1.231	1.37
47	Ag	$5s$	1.2982	1.4820	1.688	2.12
79	Au	$6s$	2.3687	3.4729	4.321	6.84

lations of the atomic energy levels. This uncertainty is about two orders of magnitude smaller than the QED corrections considered here. Of the same order (10^{-2} from the first-order QED) are the nuclear polarization corrections, which can be calculated with 10% inaccuracy for the heavy nuclei [18].

In the present paper we find, through direct calculations of the self-energy, that the estimates of the valence-electron Lamb shift in Ref. [1] were realistic. The values reach about 0.5% of the ionization potential for the heaviest s^1 elements. These QED effects are comparable with the Breit contribution to the orbital energy. They cancel about 1% of the kinetic Dirac effects for the heavy elements. The ratios of the Lamb shift to the relativistic contribution for the alkali and coinage metals at the DF level are given in Fig. 2. Note, that when Z approaches 3 from above, $-E_L$ approaches one-tenth of the kinetic relativistic effects.

For estimating the Lamb shift of valence ns levels in atoms or molecules, the present direct calculation supports the earlier recipe of using the Uehling potential, expressed in closed parametrized form [1], multiplied by the known ratio [2,11] $(E_{\mathrm{VP}}+E_{\mathrm{SE}})/E_{\mathrm{VP}}$ for hydrogenlike atoms.

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APPENDIX: ELECTRON WAVE FUNCTION

The Dirac-Fock approximation is well known. We used the program of Desclaux [19]. The DF ns eigenvalue $-\varepsilon_{\mathrm{DF}}$ is smaller than the experimental first ionization potential I_1. The DF valence-shell results could be reproduced by an effective local potential. Another option is to use the DS approximation. Then the Slater exchange parameter can be used to match the $\varepsilon_{\mathrm{DF}}$ or $-I_1$ for $\varepsilon_{\mathrm{DS}}(\alpha_x)$. These DS results can also be reproduced using the parameters of Salvat *et al.* [10]. The DF, DS ($\varepsilon_{\mathrm{DF}}$), and DS ($-I_1$) approximations are called (1), (2), and (3) respectively [20].

These three $5s$ wave functions for Rb are shown in Fig. 3. Around 0.001 a.u., (3) is largest, followed by (2) and (1). In the middle range ($2s$- and $3s$-like parts) the DS curves (3) and (2) have much higher amplitudes than the DF curve (1).

Further insight to the VP contribution can be obtained by considering the kinetic relativistic effects to it. The Dirac-Fock–Hartree-Fock VP ratios are shown in Table VII. Because the VP arises from distances of the order of 1×10^{-3} a.u., the relativistic effects on it should be between the magnetic dipole ($M1$) hyperfine interaction and the isomer shift ones (S'). $M1$ arises from distances of the order of $1/(2Z)$ [21], and the isomer shift from the nuclear surface. This expectation is borne out by the data in Table VII. We also see that S' would be too large for the present purpose.

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